PHYS479/879

(SH1 - Two Level Atoms, Density Matrix Theory and Optical Bloch Equations)

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Winter Term, 2024

Outline

- QM of EM-field excited two level systems
- Pauli operators
- System-bath interactions (decay/dissipation processes)
- Density operator and density matrix
- Optical Bloch equations (rotating wave approximation)
- Optical Bloch equations (no rotating wave approximation)

Coherent dynamics of a quantum two-level system (TLS)

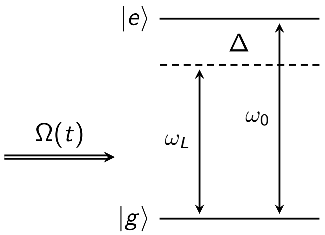


Figure: Consider a TLS interacting with a classical laser field with Rabi frequency $\Omega(t) = \mathbf{d} \cdot \mathbf{E}(t)/\hbar$.

"System" Hamiltonian of interest, using a dipole interaction between the field and TLS:

$$\boxed{H_S = H_0 + H_{\rm Int} = \hbar\omega_0 \left|e\right\rangle \left\langle e\right| + \hbar\Omega(t)(\left|e\right\rangle \left\langle g\right| + \left|g\right\rangle \left\langle e\right|)} \tag{1}$$

Pauli Operators

For TLSs, it is useful to use Pauli operators:

$$\sigma^{+} \equiv |e\rangle \langle g| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\ \sigma^{-} \equiv |g\rangle \langle e| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},\ \sigma^{+}\sigma^{-} \equiv \sigma_{ee} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\sigma^{-}\sigma^{+} \equiv \sigma_{gg} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},\ \ \sigma^{+}\sigma^{-} + \sigma^{-}\sigma^{+} = \mathbf{1},\ \ \sigma^{+}\sigma^{-} - \sigma^{-}\sigma^{+} = \sigma^{z}$$

Thus we can write:

$$\boxed{H_S = \hbar\omega_0\sigma^{+}\sigma^{-} + \hbar\Omega(t)(\sigma^{+} + \sigma^{-})} \tag{2}$$

$$\texttt{Rabi Frequency}:\ \Omega(t) \equiv \frac{\mathbf{d}\cdot\mathbf{E}(t)}{\hbar}, \tag{3}$$

where **d** is the dipole moment (assumed real).

TLS-Field Interaction (semiclassical - field is *classical*)

Operator for electric dipole:

$$\hat{\boldsymbol{\mu}} = -e\hat{\mathbf{x}} \tag{4}$$

Dipole matrix element for TLS (assumed real):

$$\mathbf{d}_{eg} = e\,\langle \mathrm{e}|\hat{\mathbf{x}}|\mathrm{g}\rangle = e\,\langle \mathrm{g}|\hat{\mathbf{x}}|\mathrm{e}\rangle \equiv \mathbf{d} \tag{5}$$

We can write in terms of Pauli operators:

$$\hat{\boldsymbol{\mu}} = -(\sigma^{+} + \sigma^{-})\mathbf{d} \tag{6}$$

Atom-field interaction Hamiltonian:

$$\boxed{H_{\mathrm{Int}} = -\hat{\boldsymbol{\mu}} \cdot \mathbf{E}(\mathbf{r}_0) = \mathbf{d} \cdot \mathbf{E}\,(\sigma^{+} + \sigma^{-}) = \hbar\Omega(t)\,(\sigma^{+} + \sigma^{-})} \tag{7}$$

Rabi frequency:

$$\Omega(t) \equiv \frac{\mathbf{d} \cdot \mathbf{E}(t)}{\hbar} \tag{8}$$

Three common pictures of quantum mechanics

From Wikipedia:

Summary comparison of evolution in all pictures [edit]

For a time-independent Hamiltonian H_S, where $H_{0,S}$ is the free Hamiltonian,

Evolution of:	Picture (v · t · e)		
	Schrödinger (S)	Heisenberg (H)	**Interaction** (I)
Ket state	$\vert\psi_S(t)\rangle = e^{-iH_S\ t/\hbar}\vert\psi_S(0)\rangle$	constant	$\vert\psi_I(t)\rangle = e^{iH_{0,S}\ t/\hbar}\vert\psi_S(t)\rangle$
Observable	constant	$A_H(t) = e^{iH_S\ t/\hbar}A_S e^{-iH_S\ t/\hbar}$	$A_I(t) = e^{iH_{0,S}\ t/\hbar}A_S e^{-iH_{0,S}\ t/\hbar}$
Density matrix	$\rho_S(t) = e^{-iH_S\ t/\hbar}\rho_S(0)e^{iH_S\ t/\hbar}$	constant	$\rho_I(t) = e^{iH_{0,S}\ t/\hbar}\rho_S(t)e^{-iH_{0,S}\ t/\hbar}$

Figure: Three "pictures" of quantum dynamics.

The interaction picture is the most common one for describing light-matter interactions, and the dynamics of TLS, qubits (quantum bits), etc.

Interaction Picture

For convenience when making approximations, one can use the *interaction picture* of QM, at the frame of the laser frequency ($H_0 = \hbar\omega_L \sigma^+\sigma^-$).

$$\boxed{\tilde{\hat{O}}(t) = e^{iH_0 t/\hbar}\hat{O}(0)e^{-iH_0 t/\hbar}} \,, \tag{9}$$

or can obtain from $\dot{\hat{O}} = \frac{i}{\hbar}[H_0, \hat{O})]$ (Heisenberg picture).

$$\text{Using } \mathbf{E}(t) = \frac{1}{2}\mathbf{E}_0(t)(e^{i\omega_L t} + e^{-i\omega_L t}) \,, \tag{10}$$

we can derive

$$\boxed{\tilde{H}_S = \hbar(\omega_0 - \omega_L)\sigma^+\sigma^- + \tilde{\Omega}_0(t)[\sigma^+(1 + e^{i2\omega_L t}) + \sigma^-(1 + e^{-i2\omega_L})]} \,, \tag{11}$$

with $\tilde{\Omega}(t) = \Omega_0(t) = \mathbf{d} \cdot \mathbf{E}(t)/(2\hbar)$, the "slowly-varying envelope".

Rotating Wave Approximation (RWA) and CW Fields

In a RWA, we neglect the fast oscillations that rotate at almost two times the TLS or laser frequency (assume average to zero), so that:

$$\boxed{\tilde{H}_S = \hbar(\omega_0 - \omega_L)\sigma^+\sigma^- + \tilde{\Omega}_0(t)(\sigma^+ + \sigma^-)} \tag{12}$$

This is expected to be valid when:

- $|(\omega_0 - \omega_L)| \ll (\omega_L + \omega_L)$ or $|(\omega_0 - \omega_L)| \ll (\omega_L + \omega_0)$
- $|\Omega(t)| \ll \omega_0$

For a continuous wave (CW) field, then:

- $\tilde{\Omega}_0(t) = \Omega_0$ (e.g., a monochromatic laser) ,

and we have a time-independent problem! This is a huge advantage of using the interaction picture.

Summary: Coherent System Hamiltonian for Excited TLS

Using the common RWA, we would solve

$$\boxed{\tilde{H}_s = \hbar(\omega_0 - \omega_L)\sigma^+\sigma^- + \hbar\tilde{\Omega}(t)(\sigma^+ + \sigma^-)\ ,} \tag{13}$$

where $\tilde{\Omega}(t)$ is usually a laser pulse, such as a Gaussian time pulse:

$$\tilde{\Omega}(t) = \Omega_0 \exp\left(-t^2/t_p^2\right), \tag{14}$$

and t_p is the pulse duration.

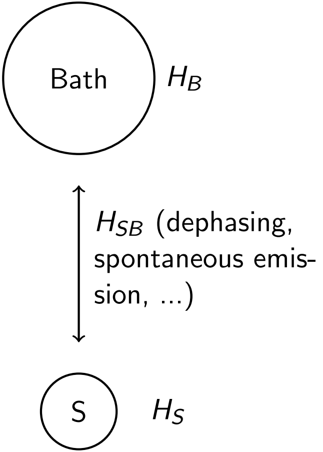
Using a full-wave pulse (i.e., no RWA), then we have

$$\boxed{H_s = \hbar\omega_0\sigma^+\sigma^- + \hbar\Omega(t)(\sigma^+ + \sigma^-)\ ,} \tag{15}$$

where $\Omega(t)$ is a full-wave Rabi field:

$$\Omega(t) = \Omega_0 \exp\left(-t^2/t_p^2\right)\sin(\omega_L t + \phi) \tag{16}$$

Dephasing Processes and System-Bath Interactions



In real systems, we have a complex problem to solve with many degrees of freedom:

$$H = H_S + H_B + H_{SB} \tag{17}$$

$$\boxed{\begin{aligned} H_S &= \hbar\omega_0 \sigma^+ \sigma^- \\ H_B &= \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k \\ H_{SB} &= \sum_k \hbar g_k (\sigma^+ + \sigma^-)(\hat{a}_k^\dagger + \hat{a}_k) \end{aligned}} \tag{18}$$

Pure States versus Mixed States

- Just like we need statistical ideas on complicated classical systems (e.g., many degrees of freedom, collections of atoms), we also need statistical ideas in QM.
- The density operator or density matrix is one of the most important tools in QM that allows one to connect QM to Stat Mech, and describe realistic systems.
- Example Pure State: $|\psi\rangle = a_g |g\rangle + a_e |e\rangle$. The only randomness here is related to measurements, e.g., $|a_g|^2$ is the probability of measuring state $|g\rangle$.
- Example Mixed State: consider a mixture of $|I\rangle = \frac{1}{\sqrt{2}}(|g\rangle - |e\rangle)$ (probability P_1) and $|II\rangle = \frac{1}{\sqrt{2}}(|g\rangle + |e\rangle)$ (probability P_2). Then the ensemble average of an expectation value, e.g., with $\sigma_{ee} = \sigma^+\sigma^-$, is

$$\boxed{\langle\sigma_{ee}\rangle = P_1 \langle\psi_I|\sigma_{ee}|\psi_I\rangle + P_2 \langle\psi_{II}|\sigma_{ee}|\psi_{II}\rangle} \equiv n_e \,(\text{population}) \quad (19)$$

Density Matrix or Density Operator

- Density matrix (DM):

$$\boxed{\rho = \sum_j P_j \left|\psi_j\right\rangle \left\langle\psi_j\right|} \tag{20}$$

– usually without a hat to stress that this is not a usual operator associated with any measurements, but rather represents a state (in general, a mixed state) for the system.
The DM is the most complete way of describing a mixed QM state, including interactions with the Baths (it is a beautiful thing!).

- Expectation of an operator:

$$\boxed{\langle \hat{O}(t)\rangle = \mathrm{Tr}[\rho(t)\hat{O}]} \tag{21}$$

which works for both pure and mixed states! (Tr: Trace).

- Liouville equation:

$$\boxed{\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}\left[H, \rho(t)\right]} \tag{22}$$

Density Matrix for a TLS and Optical Bloch Equations

The optical Bloch equations (OBEs) are one of the most accurate and celebrated approaches to describing field interactions with TLSs:

$$\rho(t) = \begin{pmatrix} \langle \sigma^+ \sigma^- \rangle & \langle \sigma^+ \rangle \\ \langle \sigma^- \rangle & \langle \sigma^- \sigma^+ \rangle \end{pmatrix} = \begin{pmatrix} n_e & \rho_{eg} \\ \rho_{ge} & n_g \end{pmatrix}$$

This gives us the following (time-dependent) "observables":

- Population of excited state: $\boxed{n_e(t)}$
- Population of ground state: $\boxed{n_g(t) = 1 - n_e(t)}$
- Coherence: $\boxed{\rho_{ge}(t) = \rho^*_{eg}(t) \equiv u(t)}$
- Macroscopic optical polarization: $\boxed{\mathbf{P}(t) = N\mathbf{d}\,\langle \boldsymbol{\mu}(t) \rangle = N\mathbf{d}2\mathrm{Re}[u(t)]}$ (N is TLS density); can connect this to Maxwell's equations.

Coherent Optical Bloch Equations (RWA)

Defining $\Delta_{0L} = \omega_0 - \omega_L$, and using a RWA, we have

$$\boxed{\tilde{H}_s = \hbar\Delta_{0L}\sigma^+\sigma^- + \hbar\tilde{\Omega}(t)(\sigma^+ + \sigma^-)} \tag{23}$$

This yields the following equations of motion:

$$\frac{du}{dt} = -i\Delta_{0L}u + i\frac{\tilde{\Omega}(t)}{2}(2n_e - 1) \tag{24}$$

$$\frac{dn_e}{dt} = -\tilde{\Omega}(t)Im[u] \tag{25}$$

which are the celebrated OBEs (Optical Bloch Equations), used to describe numerous effects with two-state systems (NMR, Rabi Oscillations, Photon Echo, Self Induced Transparency, Gain, Absorption, Lasing, ...)

Optical Bloch Equations with Dephasing (RWA)

With polarization dephasing only (e.g., due to "elastic" bath interactions):

$$\boxed{\begin{aligned} \frac{du}{dt} &= -\gamma_d u - i\Delta_{0L}u + i\frac{\tilde{\Omega}(t)}{2}(2n_e - 1) \qquad (26) \\ \frac{dn_e}{dt} &= -\tilde{\Omega}(t)Im[u] \qquad (27) \end{aligned}}$$

With spontaneous emission (SE) processes, e.g., due to interaction with photonic baths and vacuum field fluctuations, with SE decay rate γ, then

$$\boxed{\begin{aligned} \frac{du}{dt} &= -\frac{\gamma}{2}u - i\Delta_{0L}u + i\frac{\tilde{\Omega}(t)}{2}(2n_c - 1) \qquad (28) \\ \frac{dn_e}{dt} &= -\gamma n_e - \tilde{\Omega}(t)Im[u] \qquad (29) \end{aligned}}$$

Full-Wave Optical Bloch Equations (no RWA!)

Coherent OBEs (u is now quickly varying):

$$\boxed{\begin{aligned}\frac{du}{dt} &= -i\omega_0 u + i\Omega(t)(2n_e - 1) && (30)\\ \frac{dn_e}{dt} &= -2\Omega(t)Im[u] && (31)\end{aligned}}$$

With polarization dephasing, then:

$$\boxed{\begin{aligned}\frac{du}{dt} &= -\gamma_d u - i\omega_0 u + i\Omega(t)(2n_e - 1) && (32)\\ \frac{dn_e}{dt} &= -2\Omega(t)Im[u] && (33)\end{aligned}}$$

Some Known Analytical Solutions (RWA and Coherent)

- **CW Rabi oscillations.** Assuming: $n_e(0) = 0, \tilde{\Omega} = \Omega_0, \Delta_{0L} = 0$, then

$$\boxed{\begin{aligned} n_e(t) &= \sin^2(\Omega_0 t) \\ n_g(t) &= \cos^2(\Omega_0 t) \end{aligned}} \tag{34}$$

- **Pulsed Rabi oscillations and "Area Theorem".** The pulse area:

$$\boxed{A_{\rm pulse} = \int_{-\infty}^{\infty} dt\, \tilde{\Omega}(t)} \tag{35}$$

  will produce exactly n Rabi cycles of the population for a $m\ 2\pi$ pulse (m = 1,2,3, ...).

- A 2π pulse will excite from the ground state to the excited state and back again (for any pulse width). This yields temporal solitons.